THE CALCULATION OF INTERPLANAR SPACINGS OF CRYSTAL SYSTEMS BY VECTORS.

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ABSTRACT. Expressions for the calculation of interplanar spacings of crystal systems: cubic, simple tetragonal, simple orthorhombic, hexagonal, simple monoclinic, triclinic and rhombohedral have been derived by vectors. This treatment is shown to be much briefer and simpler than the one given by analytical methods, which are generally employed at present for these derivations.

The method of calculating the interplanar spacings between the successive planes in any assumed crystal structure is based at present on a well-known theorem in solid analytic geometry, which gives the perpendicular distance d from any point to a plane. The derivations of the expression for d by this method, especially for lattices other than cubic, seem to be accompanied by analytical complexities. We shall derive these expressions here by vectors, which make the derivations much briefer and simpler than the analytical method.

The perpendicular distance d_{hkl} between the successive planes of a given set may be expressed as a function of the lattice constants a_o, b_o, and c_o, and of the Miller indices (hkl) of the set of planes in question as follows.

Let OX, OY and OZ be the crystal axes: a_o be the unit distance along OX, b_o along OY and c_o along OZ, and $\bar{\mathbf{a}}$, $\bar{\mathbf{b}}$ and $\bar{\mathbf{c}}$ be the unit vectors along the axes respectively. Let $\bar{\mathbf{n}}$ be the unit vector normal to plane (hkl), then,

$$\bar{\mathbf{n}}=n_a\,\bar{\mathbf{a}}+n_b\,\bar{\mathbf{b}}+n_c\,\bar{\mathbf{c}} \qquad \dots \quad (1)$$

$$(\bar{\mathbf{n}}\,\bar{\mathbf{a}})\frac{a_o}{h}=(\bar{\mathbf{n}}.\bar{\mathbf{b}})\frac{b_o}{k}=(\bar{\mathbf{n}}.\,\bar{\mathbf{c}})\frac{c_o}{l}=d \qquad \dots \quad (2)$$

$$\bar{\mathbf{n}}.\,\bar{\mathbf{n}}=1 \qquad \dots \quad (3)$$

I. *Cubic, simple tetragonal and orthorhombic lattices:*

For these lattices,

$$\alpha=\beta=\gamma=90^\circ$$

then,

$$\bar{\mathbf{a}}\,.\,\bar{\mathbf{b}}=\bar{\mathbf{a}}\,.\,\bar{\mathbf{c}}=\bar{\mathbf{b}}\,.\,\bar{\mathbf{c}}=0 \qquad \dots \quad (4)$$

and

$$\bar{\mathbf{a}}\,.\,\bar{\mathbf{a}}=\bar{\mathbf{b}}\,.\,\bar{\mathbf{b}}=\bar{\mathbf{c}}\,.\,\bar{\mathbf{c}}=1. \qquad \dots \quad (5)$$

Substituting for $\bar{n}$ in equations (2) and (3), the right hand side of equation (1), one obtains,

$$n_a(\bar{a}.\bar{a})\frac{a_o}{h} = n_b(\bar{b}.\bar{b})\frac{b_o}{k} = n_c(\bar{c}.\bar{c})\frac{c_o}{l} = d$$

or

$$n_a\frac{a_o}{h} = n_b\frac{b_o}{k} = n_c\frac{c_o}{l} = d \qquad \dots \quad (6)$$

and

$$(n_a)^2 + (n_b)^2 + (n_c)^2 = 1. \qquad \dots \quad (7)$$

Solving equation (6)

$$n_a = \frac{d}{a_o} h$$

$$n_b = \frac{d}{b_o} k$$

$$n_c = \frac{d}{c_o} l$$

Substituting the values of n_a, n_b, and n_c in equation (7) we get

$$\frac{d^2}{a_o} h^2 + \frac{d^2}{b_o} k^2 + \frac{d^2}{c_o} l^2 = 1.$$

Solving for d or d_{hkl}.

$$d_{hkl} = \frac{1}{\sqrt{\frac{h^2}{a_o^2} + \frac{k^2}{b_o^2} + \frac{l^2}{c_o^2}}} \qquad \dots \quad (8)$$

(*a*) For a cubic lattice, $a_o = b_o = c_o$, therefore

$$d_{hkl} = \frac{a_o}{\sqrt{h^2+k^2+l^2}}. \qquad \dots \quad (9)$$

(*b*) For a simple tetragonal lattice, $a_o = b_o \neq c_o$, therefore

$$d_{hkl} = \sqrt{\frac{a_o}{h^2+k^2+\frac{a_o^2}{c_o} l^2}} = \sqrt{\frac{a_o}{h^2+k^2+\frac{l^2}{c^2}}}\ . \qquad \dots \quad (10)$$

The ratio of two units of length $c_o/a_o = c$ is called the "axial ratio."

(c) For a simple orthorhombic lattice $a_o \neq b_o \neq c_o$, therefore

$$d_{hkl} = \frac{b_o}{\sqrt{\frac{b_o^2}{a_o} h^2 + k^2 + \frac{b_o^2}{c_o} l_2}}.$$

or

$$d_{hkl} = \frac{b_o}{\sqrt{\frac{h^2}{a^2} + k^2 + \frac{l^2}{c^2}}} \qquad \ldots \quad (11)$$

where $a_o/b_o = a$, and $c_o/b_o = c$ are the axial ratios.

II. *Hexagonal Lattice* :

For a hexagonal lattice, $a_o = b_o \neq c_o$, and $\alpha = \beta = 90°$, $\gamma = 120°$, then

$$\bar{a} \,.\, \bar{b} = -\frac{1}{2},\ \bar{a} \,.\, \bar{c} = \bar{b} \,.\, \bar{c} = 0 \qquad \ldots \quad (12)$$

From equations (1), (2) and (3) subject to the conditions in equation (12) one obtains as before,

$$n_a \frac{a_o}{h} - \frac{1}{2} n_b \frac{a_o}{h} = d \qquad \ldots \quad (13)$$

$$-\frac{1}{2} n_a \frac{b_o}{k} + n_b \frac{b_o}{k} = d \qquad \ldots \quad (14)$$

$$n_c \frac{c_o}{l} = d \qquad \ldots \quad (15)$$

and

$$(n_a)^2 + (n_b)^2 + (n_c)^2 - n_a n_b = 1. \qquad \ldots \quad (16)$$

Solving equations (13), (14) and (15)

$$n_a = \frac{2}{3} \frac{d}{a_o} (2h + k)$$

$$n_b = \frac{2}{3} \frac{d}{b_o} (h + 2k)$$

$$n_c = \frac{d}{c_o} l.$$

Substituting the values of n_a, n_b and n_c in equation (16), we get

$$d^2 \left\{ \frac{4}{9a_o^2} (2h+k)^2 + \frac{4}{9b_o^2} (h+2k)^2 + \frac{l^2}{c_o^2} - \frac{4}{9a_o b_o} (2h+k)\ (h+2k) \right\} = 1.$$

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Since, for the hexagonal system $a_o = b_o \neq c_o$, therefore,

$$d^2\left\{\frac{4}{9a_o^2}(5h^2+8hk+5k^2)-\frac{4}{9a_o^2}(2h^2+5hk+2k^2)+\frac{l^2}{c_o^2}\right\}=1$$

or

$$d^2\left\{\frac{4}{3a_o^2}(h^2+hk+k^2)+\frac{l^2}{c_o^2}\right\}=1.$$

Solving for d or d_{hkl}, we get

$$d_{hkl}=\sqrt{\frac{a_o}{\frac{4}{3}(h^2+hk+k^2)+\left(\frac{a_o}{c_o}\right)l^2}}$$

or

$$d_{hkl}=\sqrt{\frac{a_o}{\frac{4}{3}(h^2+hk+k^2)+\frac{l^2}{c^2}}} \qquad \ldots \quad (17)$$

III. *Simple Monoclinic Lattice*:

For a simple monoclinic lattice, $a_o \neq b_o \neq c_o$,

$\alpha=\gamma=90°$, and $\beta \neq 90°$, then

$$\bar{a}.\,\bar{c}=\cos\beta,\quad \bar{a}.\,\bar{b}=\bar{b}.\,\bar{c}=0. \qquad \ldots \quad (18)$$

From equations (1), (2) and (3) subject to conditions in equation (18), we get

$$n_a\frac{a_o}{h}+n_c\frac{a_o}{h}\cos\beta=d \qquad \ldots \quad (19)$$

$$n_b\frac{b_o}{k}=d \qquad \ldots \quad (20)$$

$$n_a\frac{c_o}{l}\cos\beta+n_c\frac{c_o}{l}=d \qquad \ldots \quad (21)$$

and

$$(n_a)^2+(n_b)^2+(n_c)^2+2n_an_c\cos\beta=1 \qquad \ldots \quad (22)$$

Solving equations (19), (20) and (21),

$$n_a=\frac{d}{\sin^2\beta}\left(\frac{h}{a_o}-\frac{l}{c_o}\cos\beta\right)$$

$$n_b=\frac{d}{b_o}k$$

$$n_c=\frac{c}{\sin^2\beta}\left(\frac{l}{c_o}\;\frac{h}{a_o}\cos\beta\right),$$

Substituting the values of n_a, n_b and n_c in the equation (22), we get

$$d^2\left[\frac{1}{\sin^2\beta}\left\{\left(\frac{h}{a_o}\right)^2+\left(\frac{l}{c_o}\right)^2-\frac{2hl}{a_o c_o}\cos\beta\right\}+\left(\frac{k}{b_o}\right)^2\right]=1.$$

Solving for d or d_{hkl},

$$d_{hkl}=\frac{b_o}{\sqrt{\dfrac{\left(\frac{h}{a}\right)^2+\left(\frac{l}{c}\right)^2-\frac{2hl}{ac}\cos\beta}{\sin^2\beta}+k^2}} \qquad \dots \quad (23)$$

IV. *Triclinic Lattice*:

For the triclinic lattice, $a_o \neq b_o \neq c_o$, and $\alpha\neq\beta\neq\gamma\neq 90°$, then

$$\bar{\mathbf{a}}\,.\,\bar{\mathbf{b}}=\cos\gamma,\ \bar{\mathbf{a}}\,.\,\bar{\mathbf{c}}=\cos\beta,\text{ and }\ \bar{\mathbf{b}}\,.\,\bar{\mathbf{c}}=\cos\alpha \qquad \dots \quad (24)$$

From equations (1) and (2) we obtain

$$n_a\frac{a_o}{h}+n_b(\bar{\mathbf{a}}\,.\,\bar{\mathbf{b}})\frac{a_o}{h}+n_c(\bar{\mathbf{a}}\,.\,\bar{\mathbf{c}})\frac{a_o}{h}=d \qquad \dots \quad (25)$$

$$n_a(\bar{\mathbf{a}}\,.\,\bar{\mathbf{b}})\frac{b_o}{k}+n_b\,.\,\frac{b_o}{k}+n_c(\bar{\mathbf{b}}\,.\,\bar{\mathbf{c}})\frac{b_o}{k}=d \qquad \dots \quad (26)$$

and
$$n_a(\bar{\mathbf{a}}.\bar{\mathbf{c}})\frac{b_o}{k}+n_b(\bar{\mathbf{b}}.\,\bar{\mathbf{c}})\frac{c_o}{l}+n_c\frac{c_o}{l}=d \qquad \dots \quad (27)$$

Substituting the values of $\bar{\mathbf{a}}.\,\bar{\mathbf{b}}$, $\bar{\mathbf{a}}.\,\bar{\mathbf{c}}$, and $\bar{b}.\,\bar{\mathbf{c}}$ from equation (24) in equations (25), (26) and (27), and simplifying, we get

$$n_a+n_b\cos\gamma+n_c\cos\beta=\frac{d}{a_o}\,h \qquad \dots \quad (28)$$

$$n_a\cos\gamma+n_b+n_c\cos\alpha=\frac{d}{b_o}\,k \qquad \dots \quad (29)$$

$$n_a\cos\beta+n_b\cos\alpha+n_c=\frac{d}{c_o}\,l \qquad \dots \quad (30)$$

Solving equations (28), (29) and (30) for n_a, n_b and n_c by the method of determinants, we get

$$n_a = \frac{\begin{vmatrix} d\frac{h}{a_0} & \cos\gamma & \cos\beta \\ d\frac{k}{b_0} & 1 & \cos\alpha \\ d\frac{l}{c_0} & \cos\alpha & 1 \end{vmatrix}}{\begin{vmatrix} 1 & \cos\gamma & \cos\beta \\ \cos\gamma & 1 & \cos\alpha \\ \cos\beta & \cos\alpha & 1 \end{vmatrix}}$$

$$n_b = \frac{\begin{vmatrix} 1 & d\frac{h}{a_0} & \cos\beta \\ \cos\gamma & d\frac{k}{b_0} & \cos\alpha \\ \cos\beta & d\frac{l}{c_0} & 1 \end{vmatrix}}{\begin{vmatrix} 1 & \cos\gamma & \cos\beta \\ \cos\gamma & 1 & \cos\alpha \\ \cos\beta & \cos\alpha & 1 \end{vmatrix}}$$

$$n_c = \frac{\begin{vmatrix} 1 & \cos\gamma & d\frac{h}{a_0} \\ \cos\gamma & 1 & d\frac{k}{b_0} \\ \cos\beta & \cos\alpha & d\frac{l}{c_0} \end{vmatrix}}{\begin{vmatrix} 1 & \cos\gamma & \cos\beta \\ \cos\gamma & 1 & \cos\alpha \\ \cos\beta & \cos\alpha & 1 \end{vmatrix}}$$

From equation (3) it follows :

$$\bar{n}.(n_a\bar{a}+n_b\bar{b}+n_c\bar{c})=1$$

or

$$(\bar{n}.\bar{a})n_a + (\bar{n}.\bar{b})n_b + (\bar{n}.\bar{c})n_c = 1. \qquad \dots (31)$$

From equation (2) one obtains

$$\bar{n}\,.\,\bar{a} = d\frac{h}{a_o},\quad \bar{n}\,.\,\bar{b} = d\frac{k}{b_o},\ \text{and}\ \bar{n}\,.\,\bar{c} = d\frac{l}{c_o}.$$

Substituting the values of $\bar{n}\,.\,\bar{a}$, $\bar{n}\,.\,\bar{b}$, $\bar{n}\,.\,\bar{c}$, n_a, n_b and n_c as obtained above, in equation (31), we get

$$\frac{d\dfrac{h}{a_0}\begin{vmatrix} d\dfrac{h}{a_o} & \cos\gamma & \cos\beta \\ d\dfrac{k}{b_o} & 1 & \cos\alpha \\ d\dfrac{l}{c_o} & \cos\alpha & 1 \end{vmatrix} + d\dfrac{k}{b_o}\begin{vmatrix} 1 & d\dfrac{h}{a_o} & \cos\beta \\ \cos\gamma & d\dfrac{k}{b_o} & \cos\alpha \\ \cos\beta & d\dfrac{l}{c_o} & 1 \end{vmatrix} + \dfrac{dl}{c_o}\begin{vmatrix} 1 & \cos\gamma & d\dfrac{h}{a_o} \\ \cos\gamma & 1 & d\dfrac{k}{b_o} \\ \cos\beta & \cos\alpha & d\dfrac{l}{c_o} \end{vmatrix}}{\begin{vmatrix} 1 & \cos\gamma & \cos\beta \\ \cos\gamma & 1 & \cos\alpha \\ \cos\beta & \cos\alpha & 1 \end{vmatrix}} = 1 \qquad \dots (32)$$

This may be simplified to

$$\frac{\left\{\dfrac{d}{b_o}\right\}^2\dfrac{h}{a}\begin{vmatrix} \dfrac{h}{a} & \cos\gamma & \cos\beta \\ k & 1 & \cos\alpha \\ \dfrac{l}{c} & \cos\alpha & 1 \end{vmatrix} + \left\{\dfrac{d}{b_o}\right\}^2 k\begin{vmatrix} 1 & \dfrac{h}{a} & \cos\beta \\ \cos\gamma & k & \cos \\ \cos\beta & \dfrac{l}{c} & 1 \end{vmatrix} + \left\{\dfrac{d}{b_o}\right\}^2\dfrac{l}{c}\begin{vmatrix} 1 & \cos\gamma & \dfrac{h}{a} \\ \cos\gamma & 1 & k \\ \cos\beta & \cos\alpha & \dfrac{l}{c} \end{vmatrix}}{\begin{vmatrix} 1 & \cos\gamma & \cos\beta \\ \cos\gamma & 1 & \cos\alpha \\ \cos\beta & \cos\alpha & 1 \end{vmatrix}} = 1$$

Solving for d or d_{hkl},

$$d_{hkl}=\frac{b_0}{\sqrt{\dfrac{\dfrac{h}{a}\begin{vmatrix}\dfrac{h}{a} & \cos\gamma & \cos\beta\\ k & 1 & \cos\alpha\\ \dfrac{l}{c} & \cos\alpha & 1\end{vmatrix}+k\begin{vmatrix}1 & \dfrac{h}{a} & \cos\beta\\ \cos\gamma & k & \cos\alpha\\ \cos\beta & \dfrac{l}{c} & 1\end{vmatrix}+\dfrac{l}{c}\begin{vmatrix}1 & \cos\gamma & \dfrac{h}{a}\\ \cos\gamma & 1 & k\\ \cos\beta & \cos\alpha & \dfrac{l}{c}\end{vmatrix}}{\begin{vmatrix}1 & \cos\gamma & \cos\beta\\ \cos\gamma & 1 & \cos\alpha\\ \cos\beta & \cos\alpha & 1\end{vmatrix}}}} \quad \ldots \quad (33)$$

(d) For the rhombohedral lattice, $a_o=b_o=c_o$, and $\alpha=\beta=\gamma\neq 90°$. Then,

$$\bar{\mathbf{a}}\,.\,\bar{\mathbf{b}}=\bar{\mathbf{a}}\,.\,\bar{\mathbf{c}}=\bar{\mathbf{b}}\,.\,\bar{\mathbf{c}}=\cos\alpha. \quad \ldots \quad (34)$$

When these values are substituted in question (32), it becomes

$$\frac{\left(\dfrac{d}{a_o}\right)^2 h\begin{vmatrix}h & \cos\alpha & \cos\alpha\\ k & 1 & \cos\alpha\\ l & \cos\alpha & 1\end{vmatrix}+\left(\dfrac{d}{a_o}\right)^2 k\begin{vmatrix}1 & h & \cos\alpha\\ \cos\alpha & k & \cos\alpha\\ \cos\alpha & l & 1\end{vmatrix}+\left(\dfrac{d}{a_o}\right)^2 l\begin{vmatrix}1 & \cos\alpha & h\\ \cos\alpha & \cos\alpha & k\\ \cos\alpha & 1 & l\end{vmatrix}}{\begin{vmatrix}1 & \cos\alpha & \cos\alpha\\ \cos\alpha & 1 & \cos\alpha\\ \cos\alpha & \cos\alpha & 1\end{vmatrix}}=1$$

Solving for d or d_{hkl},

$$d_{hkl}=\frac{a_0}{\sqrt{\dfrac{h\begin{vmatrix}h & \cos\alpha & \cos\alpha\\ k & l & \cos\alpha\\ l & \cos\alpha & 1\end{vmatrix}+k\begin{vmatrix}\cos\alpha & h & \cos\alpha\\ l & k & \cos\alpha\\ \cos\alpha & e & 1\end{vmatrix}+\begin{vmatrix}\cos\alpha & \cos\alpha & h\\ l & \cos\alpha & k\\ \cos\alpha & l & l\end{vmatrix}}{\begin{vmatrix}1 & \cos\alpha & \cos\alpha\\ \cos\alpha & l & \cos\alpha\\ \cos\alpha & \cos\alpha & l\end{vmatrix}}}}$$

$$= \frac{a_0 \sqrt{1 + 2\cos^3\alpha - 3\cos^2\alpha}}{\sqrt{(h^2 + k^2 + l^2)\sin^2\alpha + 2(hk + hl + kl)(\cos^2\alpha - \cos\alpha)}} \qquad \dots 35$$

SUMMARY

Formulas for the calculation of interplanar spacings of crystal systems are derived by a vector method, which is much briefer and simpler to use than the analytical method. The results are summarized in table I :

TABLE I.

Lattice.	Characteristic.	No. of equation giving value for d_{hkl}.
I. Rectangular	$\alpha = \beta = \gamma = 90^\circ$	
a. Cubic	$a_0 = b_0 = c_0$	(9)
b. Simple tetragonal	$a_0 = b_0 \neq c_0$	(10)
c. Simple orthorhombic	$a_0 \neq b_0 \neq c_0$	(11)
II. Hexagonal	$a_0 = b_0 \neq c_0$	
	$\alpha = \beta = 90^\circ, \gamma = 120^\circ$	(17)
III. Simple monoclinic	$a_0 \neq b_0 \neq c_0$	
	$\alpha = \gamma = 90^\circ, \beta \neq 90^\circ$	(23)
IV. Triclinic	$a_0 \neq b_0 \neq c_0$	
	$\alpha \neq \beta \neq \gamma \neq 90^\circ$	(33)
V. Rhombohedral	$a_0 = b_0 = c_0$	
	$\alpha = \beta = \gamma \neq 90^\circ$	(35)

My thanks are due to Dr. D. R. Inglis and Professor A. G. Worthing for helpful discussions.

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